

Bond types:

- : Single
= : Double
T : Triple
: Triple
~ : Single or double query bond
% : An aromatic query bond

None : Any bond type; no explicit bond specified

\$: Ring bond; \$ before a bond type specifies ring bond
! : Chain or non-ring bond; ! before a bond type specifies chain bond

@ : A ring linkage and the number following it specifies the atoms position in the line, thus @1 means linked back to the first atom in the list.

Aromatic: Kekule or Arom5

Kekule: Bonds in 6-membered rings with alternate single/double bonds or perimeter bonds

Arom5: Bonds in 5-membered rings with two double bonds and a hetro atom at the apex of the ring.

MACCS 166 keys [Ref 45-47] are defined as follows:

Key Description

1 ISOTOPE
2 103 < ATOMIC NO. < 256
3 GROUP IVA,VA,VIA PERIODS 4-6 (Ge...)
4 ACTINIDE
5 GROUP IIIB,IVB (Sc...)
6 LANTHANIDE
7 GROUP VB,VIB,VIIB (V...)
8 QAAA@1
9 GROUP VIII (Fe...)
10 GROUP IIA (ALKALINE EARTH)
11 4M RING
12 GROUP IB,IIB (Cu...)
13 ON(C)C
14 S-S
15 OC(O)O
16 QAA@1
17 CTC
18 GROUP IIIA (B...)
19 7M RING
20 SI
21 C=C(Q)Q
22 3M RING
23 NC(O)O
24 N-O
25 NC(N)N
26 C\$=C(\$A)\$A
27 I
28 QCH2Q
29 P
30 CQ(C)(C)A
31 QX
32 CSN
33 NS
34 CH2=A
35 GROUP IA (ALKALI METAL)
36 S HETEROCYCLE
37 NC(O)N
38 NC(C)N
39 OS(O)O
40 S-O

41 CTN
42 F
43 QHAQH
44 OTHER
45 C=CN
46 BR
47 SAN
48 OQ(O)O
49 CHARGE
50 C=C(C)C
51 CSO
52 NN
53 QHAAAQH
54 QHAAQH
55 OSO
56 ON(O)C
57 O HETEROCYCLE
58 QSQ
59 Snot%A%A
60 S=O
61 AS(A)A
62 A\$A!A\$A
63 N=O
64 A\$A!S
65 C%N
66 CC(C)(C)A
67 QS
68 QHQH (&...)
69 QQH
70 QNQ
71 NO
72 OAAO
73 S=A
74 CH3ACH3
75 A!N\$A
76 C=C(A)A
77 NAN
78 C=N
79 NAAAN
80 NAAAN
81 SA(A)A
82 ACH2QH
83 QAAAA@1
84 NH2
85 CN(C)C
86 CH2QCH2
87 X!A\$A
88 S
89 OAAAO
90 QHAACH2A
91 QHAAACH2A
92 OC(N)C
93 QCH3
94 QN
95 NAAO
96 5M RING
97 NAAAO
98 QAAAAA@1
99 C=C
100 ACH2N
101 8M RING
102 QO
103 CL
104 QHACH2A
105 A\$A(\$A)\$A
106 QA(Q)Q
107 XA(A)A
108 CH3AAACH2A
109 ACH2O

110 NCO
111 NACH2A
112 AA(A)(A)A
113 Onot%A%A
114 CH3CH2A
115 CH3ACH2A
116 CH3AACH2A
117 NAO
118 ACH2CH2A > 1
119 N=A
120 HETEROCYCLIC ATOM > 1 (&...)
121 N HETEROCYCLE
122 AN(A)A
123 OCO
124 QQ
125 AROMATIC RING > 1
126 A!O!A
127 A\$A!O > 1 (&...)
128 ACH2AAACH2A
129 ACH2AACH2A
130 QQ > 1 (&...)
131 QH > 1
132 OACH2A
133 A\$A!N
134 X (HALOGEN)
135 Nnot%A%A
136 O=A > 1
137 HETEROCYCLE
138 QCH2A > 1 (&...)
139 OH
140 O > 3 (&...)
141 CH3 > 2 (&...)
142 N > 1
143 A\$A!O
144 Anot%A%Anot%A
145 6M RING > 1
146 O > 2
147 ACH2CH2A
148 AQ(A)A
149 CH3 > 1
150 A!A\$A!A
151 NH
152 OC(C)C
153 QCH2A
154 C=O
155 A!CH2!A
156 NA(A)A
157 C-O
158 C-N
159 O > 1
160 CH3
161 N
162 AROMATIC
163 6M RING
164 O
165 RING
166 FRAGMENTS

MACCS 322 keys set as defined in tables 1, 2 and 3 [Ref 46] include:

- o 26 atom properties of type P, as listed in Table 1
- o 32 one-atom environments, as listed in Table 3
- o 264 atom-bond-atom combinations listed in Table 4

Total number of keys in three tables is : 322

Atom symbol, X, used for 322 keys [Ref 46] doesn't refer to Halogens as it does for 166 keys. In order to keep the definition of 322 keys consistent with the published definitions, the symbol X is used to imply "others" atoms, but it's internally mapped to symbol X as defined for 166 keys during the generation of key values.

Atom properties-based keys (26):

| Key | Description |
|-----|---|
| 1 | A(AAA) or AA(A)A - atom with at least three neighbors |
| 2 | Q - heteroatom |
| 3 | Anot%not-A - atom involved in one or more multiple bonds, not aromatic |
| 4 | A(AAAA) or AA(A)(A)A - atom with at least four neighbors |
| 5 | A(QQ) or QA(Q) - atom with at least two heteroatom neighbors |
| 6 | A(QQQ) or QA(Q)Q - atom with at least three heteroatom neighbors |
| 7 | QH - heteroatom with at least one hydrogen attached |
| 8 | CH2(AA) or ACH2A - carbon with at least two single bonds and at least two hydrogens attached |
| 9 | CH3(A) or ACH3 - carbon with at least one single bond and at least three hydrogens attached |
| 10 | Halogen |
| 11 | A(-A-A-A) or A-A(-A)-A - atom has at least three single bonds |
| 12 | AAAAA@1 > 2 - atom is in at least two different six-membered rings |
| 13 | A(\$A\$A\$A) or A\$A(\$A)\$A - atom has more than two ring bonds |
| 14 | A\$A!A\$A - atom is at a ring/chain boundary. When a comparison is done with another atom the path passes through the chain bond. |
| 15 | Anot%A%Anot%A - atom is at an aromatic/nonaromatic boundary. When a comparison is done with another atom the path passes through the aromatic bond. |
| 16 | A!A!A - atom with more than one chain bond |
| 17 | A!A\$A!A - atom is at a ring/chain boundary. When a comparison is done with another atom the path passes through the ring bond. |
| 18 | A%Anot%A%A - atom is at an aromatic/nonaromatic boundary. When a comparison is done with another atom the path passes through the nonaromatic bond. |
| 19 | HETEROCYCLE - atom is a heteroatom in a ring. |
| 20 | rare properties: atom with five or more neighbors, atom in four or more rings, or atom types other than H, C, N, O, S, F, Cl, Br, or I |
| 21 | rare properties: atom has a charge, is an isotope, has two or more multiple bonds, or has a triple bond. |
| 22 | N - nitrogen |
| 23 | S - sulfur |
| 24 | O - oxygen |
| 25 | A(AA)A(A)A(AA) - atom has two neighbors, each with three or more neighbors (including the central atom). |
| 26 | CHACH2 - atom has two hydrocarbon (CH2) neighbors |

Atomic environments properties-based keys (32):

| Key | Description |
|-----|-------------|
| 27 | C(CC) |
| 28 | C(CCC) |
| 29 | C(CN) |
| 30 | C(CCN) |
| 31 | C(NN) |
| 32 | C(NNC) |
| 33 | C(NNN) |
| 34 | C(CO) |
| 35 | C(CCO) |
| 36 | C(NO) |
| 37 | C(NCO) |
| 38 | C(NNO) |
| 39 | C(OO) |
| 40 | C(COO) |
| 41 | C(NOO) |
| 42 | C(OOO) |
| 43 | Q(CC) |
| 44 | Q(CCC) |
| 45 | Q(CN) |
| 46 | Q(CCN) |
| 47 | Q(NN) |
| 48 | Q(CNN) |
| 49 | Q(NNN) |
| 50 | Q(CO) |
| 51 | Q(CCO) |

| | |
|----|--------|
| 52 | Q(NO) |
| 53 | Q(CNO) |
| 54 | Q(NNO) |
| 55 | Q(OO) |
| 56 | Q(COO) |
| 57 | Q(NOO) |
| 58 | Q(OOO) |

Note: The first symbol is the central atom, with atoms bonded to the central atom listed in parentheses. Q is any non-C, non-H atom. If only two atoms are in parentheses, there is no implication concerning the other atoms bonded to the central atom.

Atom-Bond-Atom properties-based keys: (264)

| Key | Description |
|-----|-------------|
| 59 | C-C |
| 60 | C-N |
| 61 | C-O |
| 62 | C-S |
| 63 | C-Cl |
| 64 | C-P |
| 65 | C-F |
| 66 | C-Br |
| 67 | C-Si |
| 68 | C-I |
| 69 | C-X |
| 70 | N-N |
| 71 | N-O |
| 72 | N-S |
| 73 | N-Cl |
| 74 | N-P |
| 75 | N-F |
| 76 | N-Br |
| 77 | N-Si |
| 78 | N-I |
| 79 | N-X |
| 80 | O-O |
| 81 | O-S |
| 82 | O-Cl |
| 83 | O-P |
| 84 | O-F |
| 85 | O-Br |
| 86 | O-Si |
| 87 | O-I |
| 88 | O-X |
| 89 | S-S |
| 90 | S-Cl |
| 91 | S-P |
| 92 | S-F |
| 93 | S-Br |
| 94 | S-Si |
| 95 | S-I |
| 96 | S-X |
| 97 | Cl-Cl |
| 98 | Cl-P |
| 99 | Cl-F |
| 100 | Cl-Br |
| 101 | Cl-Si |
| 102 | Cl-I |
| 103 | Cl-X |
| 104 | P-P |
| 105 | P-F |
| 106 | P-Br |
| 107 | P-Si |
| 108 | P-I |
| 109 | P-X |
| 110 | F-F |
| 111 | F-Br |
| 112 | F-Si |
| 113 | F-I |

| | |
|-----|-------|
| 114 | F-X |
| 115 | Br-Br |
| 116 | Br-Si |
| 117 | Br-I |
| 118 | Br-X |
| 119 | Si-Si |
| 120 | Si-I |
| 121 | Si-X |
| 122 | I-I |
| 123 | I-X |
| 124 | X-X |
| 125 | C=C |
| 126 | C=N |
| 127 | C=O |
| 128 | C=S |
| 129 | C=Cl |
| 130 | C=P |
| 131 | C=F |
| 132 | C=Br |
| 133 | C=Si |
| 134 | C=I |
| 135 | C=X |
| 136 | N=N |
| 137 | N=O |
| 138 | N=S |
| 139 | N=Cl |
| 140 | N=P |
| 141 | N=F |
| 142 | N=Br |
| 143 | N=Si |
| 144 | N=I |
| 145 | N=X |
| 146 | O=O |
| 147 | O=S |
| 148 | O=Cl |
| 149 | O=P |
| 150 | O=F |
| 151 | O=Br |
| 152 | O=Si |
| 153 | O=I |
| 154 | O=X |
| 155 | S=S |
| 156 | S=Cl |
| 157 | S=P |
| 158 | S=F |
| 159 | S=Br |
| 160 | S=Si |
| 161 | S=I |
| 162 | S=X |
| 163 | Cl=Cl |
| 164 | Cl=P |
| 165 | Cl=F |
| 166 | Cl=Br |
| 167 | Cl=Si |
| 168 | Cl=I |
| 169 | Cl=X |
| 170 | P=P |
| 171 | P=F |
| 172 | P=Br |
| 173 | P=Si |
| 174 | P=I |
| 175 | P=X |
| 176 | F=F |
| 177 | F=Br |
| 178 | F=Si |
| 179 | F=I |
| 180 | F=X |
| 181 | Br=Br |
| 182 | Br=Si |

| | |
|-----|-------|
| 183 | Br=I |
| 184 | Br=X |
| 185 | Si=Si |
| 186 | Si=I |
| 187 | Si=X |
| 188 | I=I |
| 189 | I=X |
| 190 | X=X |
| 191 | C#C |
| 192 | C#N |
| 193 | C#O |
| 194 | C#S |
| 195 | C#Cl |
| 196 | C#P |
| 197 | C#F |
| 198 | C#Br |
| 199 | C#Si |
| 200 | C#I |
| 201 | C#X |
| 202 | N#N |
| 203 | N#O |
| 204 | N#S |
| 205 | N#Cl |
| 206 | N#P |
| 207 | N#F |
| 208 | N#Br |
| 209 | N#Si |
| 210 | N#I |
| 211 | N#X |
| 212 | O#O |
| 213 | O#S |
| 214 | O#Cl |
| 215 | O#P |
| 216 | O#F |
| 217 | O#Br |
| 218 | O#Si |
| 219 | O#I |
| 220 | O#X |
| 221 | S#S |
| 222 | S#Cl |
| 223 | S#P |
| 224 | S#F |
| 225 | S#Br |
| 226 | S#Si |
| 227 | S#I |
| 228 | S#X |
| 229 | Cl#Cl |
| 230 | Cl#P |
| 231 | Cl#F |
| 232 | Cl#Br |
| 233 | Cl#Si |
| 234 | Cl#I |
| 235 | Cl#X |
| 236 | P#P |
| 237 | P#F |
| 238 | P#Br |
| 239 | P#Si |
| 240 | P#I |
| 241 | P#X |
| 242 | F#F |
| 243 | F#Br |
| 244 | F#Si |
| 245 | F#I |
| 246 | F#X |
| 247 | Br#Br |
| 248 | Br#Si |
| 249 | Br#I |
| 250 | Br#X |
| 251 | Si#Si |

| | |
|-----|--------|
| 252 | Si#I |
| 253 | Si#X |
| 254 | I#I |
| 255 | I#X |
| 256 | X#X |
| 257 | C\$C |
| 258 | C\$N |
| 259 | C\$O |
| 260 | C\$S |
| 261 | C\$Cl |
| 262 | C\$P |
| 263 | C\$F |
| 264 | C\$Br |
| 265 | C\$Si |
| 266 | C\$I |
| 267 | C\$X |
| 268 | N\$N |
| 269 | N\$O |
| 270 | N\$S |
| 271 | N\$Cl |
| 272 | N\$P |
| 273 | N\$F |
| 274 | N\$Br |
| 275 | N\$Si |
| 276 | N\$I |
| 277 | N\$X |
| 278 | O\$O |
| 279 | O\$S |
| 280 | O\$Cl |
| 281 | O\$P |
| 282 | O\$F |
| 283 | O\$Br |
| 284 | O\$Si |
| 285 | O\$I |
| 286 | O\$X |
| 287 | S\$S |
| 288 | S\$Cl |
| 289 | S\$P |
| 290 | S\$F |
| 291 | S\$Br |
| 292 | S\$Si |
| 293 | S\$I |
| 294 | S\$X |
| 295 | Cl\$Cl |
| 296 | Cl\$P |
| 297 | Cl\$F |
| 298 | Cl\$Br |
| 299 | Cl\$Si |
| 300 | Cl\$I |
| 301 | Cl\$X |
| 302 | P\$P |
| 303 | P\$F |
| 304 | P\$Br |
| 305 | P\$Si |
| 306 | P\$I |
| 307 | P\$X |
| 308 | F\$F |
| 309 | F\$Br |
| 310 | F\$Si |
| 311 | F\$I |
| 312 | F\$X |
| 313 | Br\$Br |
| 314 | Br\$Si |
| 315 | Br\$I |
| 316 | Br\$X |
| 317 | Si\$Si |
| 318 | Si\$I |
| 319 | Si\$X |
| 320 | I\$I |

```
321  I$X
322  X$X
```

SetSize

```
$MACCSKeys->SetSize($Size);
```

Sets size of MACCS keys and returns *MACCSKeys*. Possible values: *166* or *322*.

SetType

```
$MACCSKeys->SetType($Type);
```

Sets type of MACCS keys and returns *MACCSKeys*. Possible values: *MACCSKeysBits* or *MACCSKeysCount*.

StringifyMACCSKeys

```
$String = $MACCSKeys->StringifyMACCSKeys();
```

Returns a string containing information about *MACCSKeys* object.

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SEE ALSO

Fingerprints.pm, FingerprintsStringUtil.pm, AtomNeighborhoodsFingerprints.pm, AtomTypesFingerprints.pm, EStateIndicesFingerprints.pm, ExtendedConnectivityFingerprints.pm, PathLengthFingerprints.pm, TopologicalAtomPairsFingerprints.pm, TopologicalAtomTripletsFingerprints.pm, TopologicalAtomTorsionsFingerprints.pm, TopologicalPharmacophoreAtomPairsFingerprints.pm, TopologicalPharmacophoreAtomTripletsFingerprints.pm

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